Erratum: Semiempirical calculation of van der Waals coefficients and polarizabilities for the alkali-metal and alkaline-earth-metal atoms [Phys. Rev. A 68, 052714 (2003)]

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Erratum: Dispersion coefficients for H and He interactions with alkali-metal and alkaline-earth-metal atoms [Phys. Rev. A 68, 062710 (2003)]

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We have realized since publication that the higher-ℓ polarizabilities and dispersion coefficients are very sensitive to the representation of the ground-state wave function. The ground-state wave functions for Na and K were represented with a linear combination of Slater-type orbitals. One negative feature of a basis set expansion relates to the behavior at large distances from the nucleus. Unlike a grid based calculation, the correct asymptotics are not imposed and the larger-r part of the wave function has a weak influence on the binding energy.

The ground-state wave functions for Na and K were both 1.7×10^{-6} hartree away from convergence. There were some small but significant changes in the polarizabilities and dispersion parameters when the existing basis sets were replaced by a large Laguerre basis set. The octupole polarizabilities decreased by 3–4 %, while C_{10} for dimers involving these atoms decreased by about 1–2 %.

TABLE I. Values of the polarizabilities and dispersion coefficients (in atomic units) for systems with Na or K.

System	Property	Present	MBPT [1]	Property	Present	MBPT [1]
Na	$\alpha^{(2)}$	1879	1885	$\alpha^{(3)}$	5.552×10^{4}	5.54×10^{4}
K	$\alpha^{(2)}$	5005	5000	$\alpha^{(3)}$	1.777×10^{5}	1.77×10^{5}
Na-H	C_8	4012		C_{10}	2.916×10^{5}	
Na-Li	C_8	9.888×10^{4}	9.88×10^{4}	C_{10}	9.187×10^{6}	9.16×10^{6}
Na-Na	C_8	1.159×10^{5}	1.16×10^{5}	C_{10}	1.134×10^{7}	1.13×10^{7}
Na-K	C_8	2.240×10^{5}	2.24×10^{5}	C_{10}	2.532×10^{7}	2.53×10^{7}
Na-Rb	C_8	2.649×10^{5}	2.66×10^{5}	C_{10}	3.122×10^{7}	3.13×10^{7}
K-H	C_8	7970		C_{10}	7.345×10^{5}	
K-Li	C_8	1.955×10^{5}	1.95×10^{5}	C_{10}	2.101×10^{7}	2.10×10^{7}
K-K	C_8	4.197×10^{5}	4.20×10^{5}	C_{10}	5.374×10^{7}	5.37×10^{7}
K-Rb	C_8	4.904×10^{5}	4.93×10^{5}	C_{10}	6.534×10^{7}	6.60×10^{7}
Na-He	C_8	1328		C_{10}	9.514×10^{4}	
Na-Be	C_8	3.349×10^{4}		C_{10}	2.651×10^{6}	
Na-Mg	C_8	6.736×10^{4}		C_{10}	5.743×10^{6}	
Na-Ca	C_8	1.633×10^{5}		C_{10}	1.561×10^{7}	
Na-Sr	C_8	2.172×10^{5}		C_{10}	2.183×10^{7}	
K-He	C_8	2623		C_{10}	2.398×10^{5}	
K-Be	C_8	6.514×10^{4}		C_{10}	6.382×10^{6}	
K-Mg	C_8	1.283×10^{5}		C_{10}	1.335×10^{7}	
K-Ca	C_8	3.024×10^{5}		C_{10}	3.462×10^{7}	
K-Sr	C_8	3.980×10^{5}		C_{10}	4.753×10^{7}	

The impact upon $\alpha^{(2)}$ and C_8 was an order of magnitude smaller and the changes were largely confined to the last digit of the revised data given in Table I. The impact upon $\alpha^{(1)}$ and C_6 was insignificant.

One feature of the revised calculation is that some small but annoying discrepancies with the many body perturbation theory (MBPT) results of Porsev and Derevianko [1] have been largely eradicated. The $f^{(\ell)}$-value distrubtions for Li and Rb were not affected by this problem since the 2*s* and 5*s* orbitals for these atoms were computed with a large Laguerre basis.

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[1] S. G. Porsev and A. Derevianko, J. Chem. Phys. **119**, 844 (2003).